

Crystal structure of strontium perchlorate anhydrate, $\text{Sr}(\text{ClO}_4)_2$, from laboratory powder X-ray diffraction data

Jooeun Hyoung, Hyeon Woo Lee, So Jin Kim, Hong Rim Shin and Seung-Tae Hong*

Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu 42988, Republic of Korea. *Correspondence e-mail: st.hong@dgist.ac.kr

Received 16 January 2019

Accepted 8 March 2019

Edited by M. Weil, Vienna University of Technology, Austria

Keywords: crystal structure; powder X-ray diffraction; strontium perchlorate anhydrate; isotypism.

CCDC reference: 1901870

Supporting information: this article has supporting information at journals.iucr.org/e

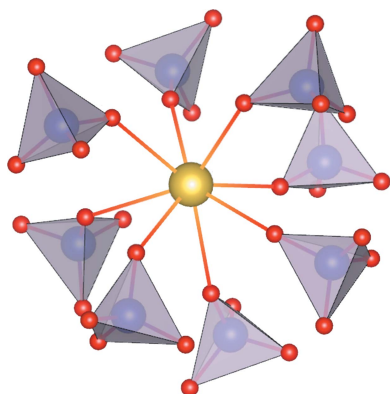
The crystal structure of strontium perchlorate anhydrate, $\text{Sr}(\text{ClO}_4)_2$, was determined and refined from laboratory powder X-ray diffraction data. The material was obtained by dehydration of $\text{Sr}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$ at 523 K for two weeks. It crystallizes in the orthorhombic space group $Pbca$ and is isotypic with $\text{Ca}(\text{AlD}_4)_2$ and $\text{Ca}(\text{ClO}_4)_2$. The asymmetric unit contains one Sr, two Cl and eight O sites, all on general positions (Wyckoff position 8c). The crystal structure consists of Sr^{2+} cations and isolated ClO_4^- tetrahedra. The Sr^{2+} cation is coordinated by eight O atoms from eight ClO_4^- tetrahedra. The validity of the crystal structure model for $\text{Sr}(\text{ClO}_4)_2$ anhydrate was confirmed by the bond valence method.

1. Chemical context

The alkaline earth metal ions (Mg^{2+} , Ca^{2+} , Sr^{2+} and Ba^{2+}) have received attention as ion carriers for next-generation batteries (Wang *et al.*, 2013), and their perchlorates are used as inorganic salts of conventional nonaqueous electrolytes for electrochemical cells in Mg- and Ca-ion batteries (Whittingham *et al.*, 2018; Tchitchekova *et al.*, 2017; Padigi *et al.*, 2015). It is crucial to obtain anhydrous salts to achieve high electrochemical cell performance since hydrated salts can cause unwanted side reactions as a result of increased water content in the nonaqueous electrolyte. Strontium perchlorate is highly hygroscopic and exists in several hydrated forms. So far, $\text{Sr}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$, $\text{Sr}(\text{ClO}_4)_2 \cdot 4\text{H}_2\text{O}$ and $\text{Sr}(\text{ClO}_4)_2 \cdot 9\text{H}_2\text{O}$ have been identified by single-crystal X-ray diffraction (Hennings *et al.*, 2014). However, the crystal structure of the anhydrous phase has not been reported to date because of the difficulty in growing single crystals. Previously, we have determined the structures of anhydrous magnesium, barium and calcium perchlorate from laboratory powder X-ray diffraction data (Lim *et al.*, 2011; Lee *et al.*, 2015, 2018). Using the same techniques for the Sr salt, we were able to determine and refine the crystal structure of strontium perchlorate anhydrate.

2. Structural commentary

The crystal structure of anhydrous strontium perchlorate, $\text{Sr}(\text{ClO}_4)_2$, is isotypic with $\text{Ca}(\text{AlD}_4)_2$ (Sato *et al.*, 2009) and $\text{Ca}(\text{ClO}_4)_2$ (Lee *et al.*, 2018). Compared with $\text{Ca}(\text{ClO}_4)_2$, the unit-cell parameters a , b and c of $\text{Sr}(\text{ClO}_4)_2$ are increased by 3.0, 2.9 and 3.4%, respectively, because Sr^{2+} (1.26 Å for eight-coordination) has a larger ionic radius than Ca^{2+} (1.12 Å for eight-coordination; Shannon, 1976).



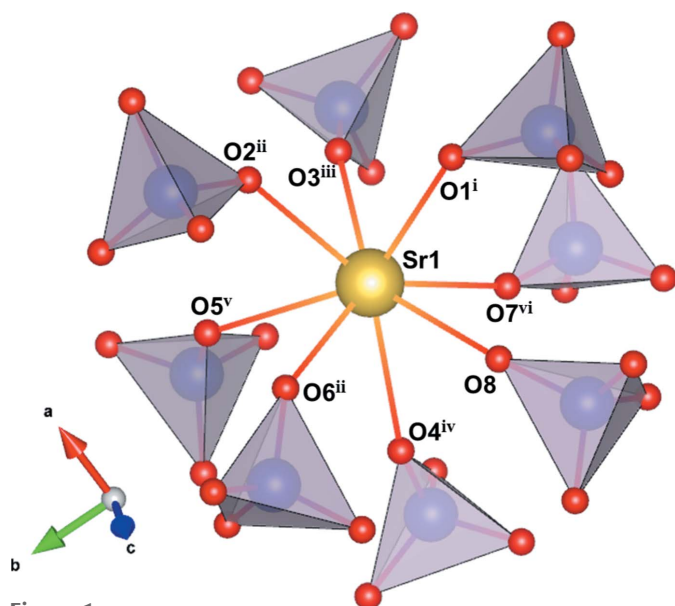


Figure 1
The local environment of the Sr^{2+} cation (yellow sphere) surrounded by ClO_4^- tetrahedra (purple). Symmetry codes refer to Table 1.

There are one Sr, two Cl and eight O sites in the asymmetric unit, all on general positions $8c$. The crystal structure (Fig. 1) is composed of Sr^{2+} cations and isolated ClO_4^- tetrahedra. The isolated ClO_4^- tetrahedra are slightly distorted and exhibit a range of $105.4(7)$ – $113.5(7)^\circ$ for the O–Cl–O angles. The local environment around the Sr^{2+} cation is presented in Fig. 2. It is coordinated by eight O atoms from eight ClO_4^- tetrahedra, with an average Sr–O distance of 2.582 \AA (Table 1). The latter is intermediate between those of Ca–O (2.476 \AA ; Lee *et al.*, 2018) and Ba–O (2.989 \AA ; Lee *et al.*, 2015) polyhedra, and in good agreement with the sum of the ionic radii of the respective alkaline earth metal and oxygen ions (Shannon, 1976).

Empirical bond valence sums (BVSs) can be used to check structure models (Brown, 2002). In this regard, the BVSs for the ions in the crystal structure of $\text{Sr}(\text{ClO}_4)_2$ were calculated with the program *Valence* (Brown & Altermatt, 1985; Brese & O’Keeffe, 1991; Hormillosa *et al.*, 1993). The expected charges of the ions match well with the obtained BVS values (given in valence units), thus confirming the validity of the crystal structure: Sr 2.18, Cl1 6.99, Cl2 6.96, O1 1.91, O2 2.08, O3 2.06, O4 2.03, O5 1.96, O6 2.02, O7 2.03 and O8 2.04.

3. Synthesis and crystallization

Anhydrous strontium perchlorate was obtained by dehydration of $\text{Sr}(\text{ClO}_4)_2 \cdot 3\text{H}_2\text{O}$ (98%, Alfa Aesar). The hydrated $\text{Sr}(\text{ClO}_4)_2$ powder was ground thoroughly in an agate mortar and added to a glass bottle. The bottle was placed in an oven at 523 K for two weeks under atmospheric conditions and then transferred to a glove-box under an argon atmosphere. For the powder X-ray diffraction measurements, anhydrous $\text{Sr}(\text{ClO}_4)_2$ was again ground in an agate mortar and placed in a tightly sealed dome-type X-ray sample holder commercially available

Table 1
Selected bond lengths (\AA).

Sr1–O1 ⁱ	2.512 (5)	Cl1–O5	1.436 (5)
Sr1–O2 ⁱⁱ	2.591 (5)	Cl1–O6	1.436 (5)
Sr1–O3 ⁱⁱⁱ	2.546 (5)	Cl1–O7	1.426 (5)
Sr1–O4 ^{iv}	2.622 (5)	Cl1–O8	1.423 (5)
Sr1–O5 ^v	2.650 (5)	Cl2–O1	1.469 (5)
Sr1–O6 ⁱⁱ	2.540 (5)	Cl2–O2	1.414 (5)
Sr1–O7 ^{vi}	2.590 (5)	Cl2–O3	1.425 (5)
Sr1–O8	2.604 (8)	Cl2–O4	1.422 (5)

Symmetry codes: (i) $x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$; (ii) $-x + 1, -y + 1, -z + 1$; (iii) $x + \frac{1}{2}, y, -z + \frac{1}{2}$; (iv) $-x + \frac{1}{2}, -y + 1, z - \frac{1}{2}$; (v) $-x + 1, y + \frac{1}{2}, -z + \frac{1}{2}$; (vi) $x, -y + \frac{1}{2}, z - \frac{1}{2}$.

from Bruker. The dome was double-sealed with vacuum grease to prevent hydration during measurement.

4. Refinement details

Details of the crystal data collection and structure refinement are summarized in Table 2. Powder X-ray diffraction (PXRD) data for anhydrous $\text{Sr}(\text{ClO}_4)_2$ were collected from a Bragg–Brentano diffractometer (PANalytical Empyrean) using

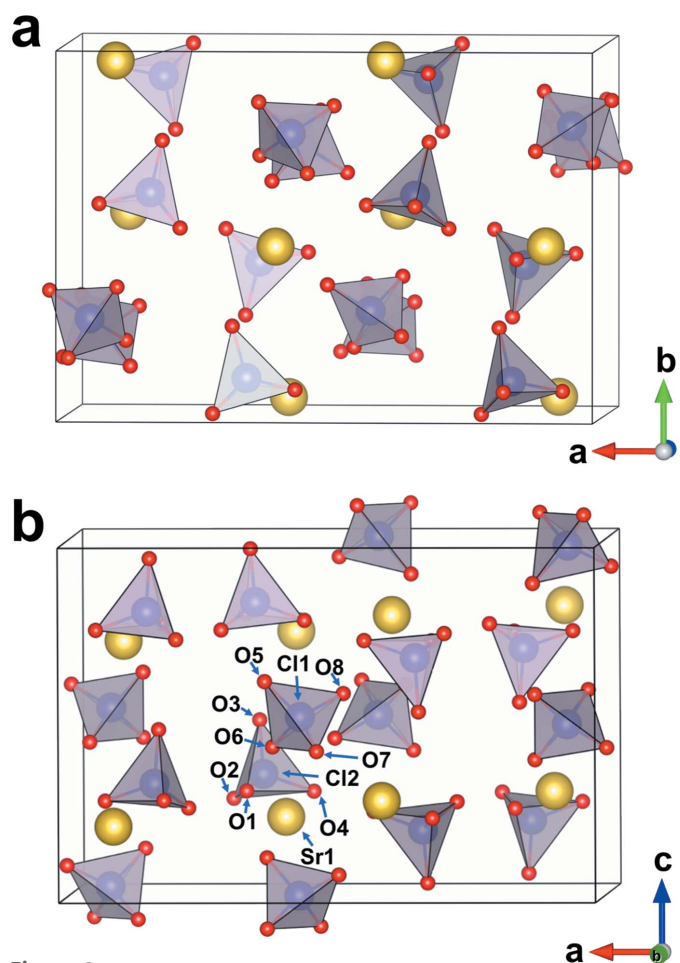


Figure 2
The crystal structure of $\text{Sr}(\text{ClO}_4)_2$ in two different viewing directions, *i.e.* approximately along (a) $[001]$ and (b) $[010]$. Sr^{2+} cations are yellow and ClO_4^- tetrahedra are purple.

Table 2
Experimental details.

Crystal data	
Chemical formula	Sr(ClO ₄) ₂
<i>M_r</i>	286.52
Crystal system, space group	Orthorhombic, <i>Pbca</i>
Temperature (K)	298
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.18206 (10), 9.78934 (11), 9.37624 (10)
<i>V</i> (Å ³)	1301.73 (2)
<i>Z</i>	8
Radiation type	Cu <i>Kα</i> ₁ , λ = 1.5405 Å
Specimen shape, size (mm)	Flat sheet, 24.9 × 24.9
Data collection	
Diffractometer	PANalytical Empyrean
Specimen mounting	Packed powder
Data collection mode	Reflection
Scan method	Step
2θ values (°)	2θ _{min} = 10.009, 2θ _{max} = 129.991, 2θ _{step} = 0.013
Refinement	
<i>R</i> factors and goodness of fit	<i>R_p</i> = 0.086, <i>R_{wp}</i> = 0.125, <i>R_{exp}</i> = 0.096, <i>R</i> (<i>F</i> ²) = 0.14871, χ ² = 1.716
No. of parameters	40
No. of restraints	23

Computer programs: *X'Pert Data Collector* (PANalytical, 2011), *GSAS* (Larson & Von Dreele, 2000), *X'Pert HighScore Plus* (PANalytical, 2011), *SHELXS97* (Sheldrick, 2008), *CRYSTALS* (Betteridge *et al.*, 2003) and *VESTA* (Momma & Izumi, 2011).

Cu *Kα*₁ radiation, a focusing primary Ge(111) monochromator (λ = 1.5406 Å) and a position-sensitive PIXcel 3D 2×2 detector. The angular range was 10 ≤ 2θ ≤ 130°, with a step of 0.0131° and a total measurement time of 8 h at room temperature. The PXRD pattern was indexed using the *TREOR90* algorithm (Werner, 1990) run in *CRYSFIRE* (Shirley, 2002) through the positions of 23 reflections, resulting in an orthorhombic unit cell. Systematic reflection conditions suggested the space group *Pbca*. The crystal structure was

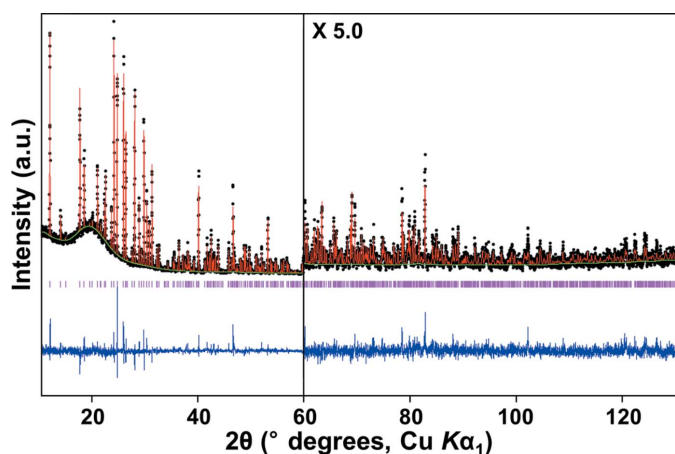


Figure 3
PXRD Rietveld refinement profiles for anhydrous Sr(ClO₄)₂ measured at ambient temperature. Black dots mark experimental data, the solid red line represents the calculated profile and the solid green line is the background. The bottom trace presents the difference curve (blue) and the ticks denote the expected Bragg reflection positions (magenta).

determined by a combination of the powder profile refinement program *GSAS* (Larson & Von Dreele, 2000) and the single-crystal structure refinement program *CRYSTALS* (Betteridge *et al.*, 2003). For a three-dimensional view of the Fourier electron-density maps, *MCE* was applied (Rohlíček & Husák, 2007). Initially, a structural model with only one dummy atom at an arbitrary position in the unit cell was used. Structure factors were extracted from the powder data and then direct methods were applied to calculate the initial solution of the crystal structure using *SHELXS97* (Sheldrick, 2008) run in *CRYSTALS*, which yielded the Sr site as a starting atomic position. The initial dummy atom model was then replaced with the partial model, and this data was adopted for a Le Bail fit in *GSAS*. Improved structure factors were then extracted, which were used for the refinement in *CRYSTALS*. Such processes were iterated until a complete and satisfactory structural model was obtained. Finally, Rietveld refinement in *GSAS* was employed to complete the structure model, resulting in reasonable isotropic displacement parameters and agreement indices. For the final Rietveld refinement with *GSAS*, the Sr—O and Cl—O bond lengths were restrained with a tolerance value of 2% with respect to the distances determined from *CRYSTALS*, which matched reasonably well with the radii sums of Shannon (1976). The final Rietveld plot is displayed in Fig. 3.

Funding information

Funding for this research was provided by: the Creative Materials Discovery Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT and Future Planning (2015M3D1A1069707).

References

- Betteridge, P. W., Carruthers, J. R., Cooper, R. I., Prout, K. & Watkin, D. J. (2003). *J. Appl. Cryst.* **36**, 1487.
- Brese, N. E. & O'Keeffe, M. (1991). *Acta Cryst.* **B47**, 192–197.
- Brown, I. D. (2002). In *The Chemical Bond in Inorganic Chemistry*. Oxford University Press.
- Brown, I. D. & Altermatt, D. (1985). *Acta Cryst.* **B41**, 244–247.
- Hennings, E., Schmidt, H. & Voigt, W. (2014). *Acta Cryst.* **E70**, 510–514.
- Hormillosa, C., Healy, S., Stephen, T. & Brown, I. D. (1993). *Bond Valence Calculator*. Version 2.0. McMaster University, Canada. http://www.CCP14.ac.uk/solution/bond_valence/.
- Larson, A. C. & Von Dreele, R. B. (2000). *General Structure Analysis System (GSAS)*. Report LAUR 86-748. Los Alamos National Laboratory, New Mexico, USA.
- Lee, D., Bu, H., Kim, D., Hyung, J. & Hong, S.-T. (2018). *Acta Cryst.* **E74**, 514–517.
- Lee, J. H., Kang, J. H., Lim, S.-C. & Hong, S.-T. (2015). *Acta Cryst.* **E71**, 588–591.
- Lim, H.-K., Choi, Y. S. & Hong, S.-T. (2011). *Acta Cryst.* **C67**, i36–i38.
- Momma, K. & Izumi, F. (2011). *J. Appl. Cryst.* **44**, 1272–1276.
- Padigi, P., Goncher, G., Evans, D. & Solanki, R. (2015). *J. Power Sources*, **273**, 460–464.
- PANalytical (2011). *X'Pert Data Collector* and *X'Pert HighScore Plus*. PANalytical BV, Almelo, The Netherlands.
- Rohlíček, J. & Husák, M. (2007). *J. Appl. Cryst.* **40**, 600–601.
- Sato, T., Sørby, M. H., Ikeda, K., Sato, S., Hauback, B. C. & Orimo, S. (2009). *J. Alloys Compd.* **487**, 472–478.

- Shannon, R. D. (1976). *Acta Cryst.* **A32**, 751–767.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Shirley, R. (2002). *The Crysfire 2002 System for Automatic Powder Indexing: User's Manual*. Guildford, UK: The Lattice Press.
- Tchitchekova, D. S., Monti, D., Johansson, P., Bardé, F., Randon-Vitanova, A., Palacín, M. R. & Pnrouch, A. (2017). *J. Electrochem. Soc.* **164**, A1384–A1392.
- Wang, R. Y., Wessells, C. D., Huggins, R. A. & Cui, Y. (2013). *Nano Lett.* **13**, 5748–5752.
- Werner, P. E. (1990). *TREOR90*. **University of?** Stockholm, Sweden.
- Whittingham, M. S., Siu, C. & Ding, J. (2018). *Acc. Chem. Res.* **51**, 258–264.

supporting information

Acta Cryst. (2019). E75, 447-450 [https://doi.org/10.1107/S2056989019003335]

Crystal structure of strontium perchlorate anhydrate, Sr(ClO₄)₂, from laboratory powder X-ray diffraction data

Joeun Hyung, Hyeon Woo Lee, So Jin Kim, Hong Rim Shin and Seung-Tae Hong

Computing details

Data collection: *X'Pert Data Collector* (PANalytical, 2011); cell refinement: *GSAS* (Larson & Von Dreele, 2000); data reduction: *X'Pert HighScore Plus* (PANalytical, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008) and *CRYSTALS* (Betteridge *et al.*, 2003); program(s) used to refine structure: *GSAS* (Larson & Von Dreele, 2000); molecular graphics: *VESTA* (Momma & Izumi, 2011); software used to prepare material for publication: *GSAS* (Larson & Von Dreele, 2000).

Strontium perchlorate anhydrate

Crystal data

Sr(ClO₄)₂

$M_r = 286.52$

Orthorhombic, *Pbca*

Hall symbol: -P_2ac_2ab

$a = 14.18206$ (10) Å

$b = 9.78934$ (11) Å

$c = 9.37624$ (10) Å

$V = 1301.73$ (2) Å³

$Z = 8$

$F(000) = 1088.0$

$D_x = 2.925$ Mg m⁻³

Cu $K\alpha_1$ radiation, $\lambda = 1.5405$ Å

$T = 298$ K

white

flat_sheet, 24.9 × 24.9 mm

Specimen preparation: Prepared at 298 K

Data collection

PANalytical Empyrean
diffractometer

Radiation source: sealed X-ray tube,
PANalytical Cu Ceramic X-ray tube

Specimen mounting: packed powder

Data collection mode: reflection

Scan method: step

$2\theta_{\min} = 10.009^\circ$, $2\theta_{\max} = 129.991^\circ$, $2\theta_{\text{step}} = 0.013^\circ$

Refinement

Least-squares matrix: full

$R_p = 0.086$

$R_{wp} = 0.125$

$R_{exp} = 0.096$

$R(F^2) = 0.14871$

9139 data points

Profile function: CW Profile function number 4

with 18 terms Pseudovoigt profile coefficients as parameterized in P. Thompson, D.E. Cox & J.B. Hastings (1987). J. Appl. Cryst.,20,79-83.

Asymmetry correction of L.W. Finger, D.E. Cox & A. P. Jephcoat (1994). J. Appl.

Cryst.,27,892-900. Microstrain broadening by P.W. Stephens, (1999). J. Appl.

Cryst.,32,281-289. #1(GU) = 0.000 #2(GV) = 0.000 #3(GW) = 0.000 #4(GP) = 9.252 #5(LX) = 0.900 #6(ptec) = 0.00 #7(trns) = 0.00 #8(shft) = -3.8100 #9(sfec) = 0.00 #10(S/L) = 0.0208

#11(H/L) = 0.0005 #12(eta) = 0.7500 #13(S400) = 0.0E+00 #14(S040) = 7.8E-04 #15(S004) = 1.5E-04 #16(S220) = 3.7E-04 #17(S202) = 6.1E-04 #18(S022) = -1.1E-03 Peak tails are ignored where the intensity is below 0.0010 times the peak Aniso. broadening axis 0.0 0.0 1.0

40 parameters

23 restraints

$(\Delta/\sigma)_{max} = 0.05$

Background function: GSAS Background

function number 1 with 34 terms. Shifted

Chebyshev function of 1st kind 1: 118.082 2:

-166.900 3: 123.865 4: -59.7925 5: 10.6865 6:

21.3336 7: -31.0975 8: 23.2200 9: -6.96687 10:

-9.51726 11: 20.8794 12: -23.8022 13: 18.4347

14: -9.14997 15: -1.10995 16: 9.35323 17:

-13.3633 18: 13.2873 19: -9.61569 20: 4.08246

21: 1.61524 22: -5.79316 23: 6.77390 24:

-5.01271 25: 2.27833 26: 0.646733 27:

-2.78842 28: 3.78393 29: -3.23100 30: 2.18997

31: -0.908158 32: -0.401332 33: 0.778547 34:

-0.792308

Preferred orientation correction: March-Dollase

AXIS 1 Ratio= 0.79858 h= 1.000 k= 0.000 l=

0.000 Preferred orientation correction range:

Min= 0.71363, Max= 1.96360

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	U_{iso}^*/U_{eq}
Sr1	0.60125 (9)	0.46444 (17)	0.2136 (2)	0.0206 (3)*
Cl1	0.4370 (3)	0.2794 (4)	0.4905 (4)	0.0254 (3)*
Cl2	0.1592 (2)	0.3965 (4)	0.6866 (4)	0.0275 (3)*
O1	0.1833 (5)	0.2549 (6)	0.7237 (14)	0.0271 (14)*
O2	0.2200 (4)	0.4878 (11)	0.7587 (12)	0.0335 (14)*
O3	0.1636 (7)	0.4175 (13)	0.5363 (6)	0.0364 (14)*
O4	0.0665 (4)	0.4250 (10)	0.7362 (11)	0.0225 (14)*
O5	0.3759 (6)	0.2145 (7)	0.3888 (11)	0.0356 (14)*
O6	0.3829 (6)	0.3692 (11)	0.5799 (10)	0.0361 (14)*

O7	0.4728 (6)	0.1764 (11)	0.5835 (12)	0.0315 (14)*
O8	0.5132 (6)	0.3514 (12)	0.4267 (12)	0.0305 (14)*

Geometric parameters (Å, °)

Sr1—Cl1	3.931 (4)	Cl2—Sr1 ^{ix}	3.945 (3)
Sr1—Cl1 ⁱ	3.937 (4)	Cl2—Sr1 ⁱⁱ	3.778 (3)
Sr1—Cl1 ⁱⁱ	3.779 (4)	Cl2—Sr1 ^x	3.746 (4)
Sr1—Cl1 ⁱⁱⁱ	3.669 (4)	Cl2—Sr1 ^{xi}	3.898 (4)
Sr1—Cl2 ^{iv}	3.945 (3)	Cl2—O1	1.469 (5)
Sr1—Cl2 ⁱⁱ	3.778 (3)	Cl2—O2	1.414 (5)
Sr1—Cl2 ^v	3.746 (4)	Cl2—O3	1.425 (5)
Sr1—Cl2 ^{vi}	3.898 (4)	Cl2—O4	1.422 (5)
Sr1—O1 ^v	2.512 (5)	O1—Sr1 ^x	2.512 (5)
Sr1—O2 ⁱⁱ	2.591 (5)	O1—Cl2	1.469 (5)
Sr1—O3 ^{vi}	2.546 (5)	O2—Sr1 ⁱⁱ	2.591 (5)
Sr1—O4 ^{iv}	2.622 (5)	O2—Cl2	1.414 (5)
Sr1—O5 ⁱⁱⁱ	2.650 (5)	O3—Sr1 ^{xi}	2.546 (5)
Sr1—O6 ⁱⁱ	2.540 (5)	O3—Cl2	1.425 (5)
Sr1—O7 ⁱ	2.590 (5)	O4—Sr1 ^{ix}	2.622 (5)
Sr1—O8	2.604 (8)	O4—Cl2	1.422 (5)
Cl1—Sr1	3.931 (4)	O5—Sr1 ^{viii}	2.650 (5)
Cl1—Sr1 ^{vii}	3.937 (4)	O5—Cl1	1.436 (5)
Cl1—Sr1 ⁱⁱ	3.779 (4)	O6—Sr1 ⁱⁱ	2.540 (5)
Cl1—Sr1 ^{viii}	3.669 (4)	O6—Cl1	1.436 (5)
Cl1—O5	1.436 (5)	O7—Sr1 ^{vii}	2.590 (5)
Cl1—O6	1.436 (5)	O7—Cl1	1.426 (5)
Cl1—O7	1.426 (5)	O8—Sr1	2.604 (8)
Cl1—O8	1.423 (5)	O8—Cl1	1.423 (5)
O1 ^v —Sr1—O2 ⁱⁱ	71.2 (3)	O5 ⁱⁱⁱ —Sr1—O8	136.8 (4)
O1 ^v —Sr1—O3 ^{vi}	84.3 (4)	O6 ⁱⁱ —Sr1—O7 ⁱ	139.7 (3)
O1 ^v —Sr1—O4 ^{iv}	138.9 (3)	O6 ⁱⁱ —Sr1—O8	74.3 (4)
O1 ^v —Sr1—O5 ⁱⁱⁱ	144.9 (3)	O7 ⁱ —Sr1—O8	78.3 (4)
O1 ^v —Sr1—O6 ⁱⁱ	109.2 (4)	O5—Cl1—O6	109.7 (5)
O1 ^v —Sr1—O7 ⁱ	88.9 (4)	O5—Cl1—O7	108.0 (7)
O1 ^v —Sr1—O8	71.3 (4)	O5—Cl1—O8	113.5 (7)
O2 ⁱⁱ —Sr1—O3 ^{vi}	77.6 (3)	O6—Cl1—O7	105.4 (7)
O2 ⁱⁱ —Sr1—O4 ^{iv}	143.6 (3)	O6—Cl1—O8	110.3 (7)
O2 ⁱⁱ —Sr1—O5 ⁱⁱⁱ	75.5 (3)	O7—Cl1—O8	109.7 (7)
O2 ⁱⁱ —Sr1—O6 ⁱⁱ	73.8 (3)	O1—Cl2—O2	110.0 (7)
O2 ⁱⁱ —Sr1—O7 ⁱ	146.3 (3)	O1—Cl2—O3	111.1 (7)
O2 ⁱⁱ —Sr1—O8	118.0 (4)	O1—Cl2—O4	108.8 (6)
O3 ^{vi} —Sr1—O4 ^{iv}	117.7 (3)	O2—Cl2—O3	110.7 (8)
O3 ^{vi} —Sr1—O5 ⁱⁱⁱ	77.9 (3)	O2—Cl2—O4	106.4 (6)
O3 ^{vi} —Sr1—O6 ⁱⁱ	141.9 (4)	O3—Cl2—O4	109.6 (6)
O3 ^{vi} —Sr1—O7 ⁱ	73.4 (3)	Sr1 ^x —O1—Cl2	139.0 (5)
O3 ^{vi} —Sr1—O8	142.8 (4)	Sr1 ⁱⁱ —O2—Cl2	139.4 (5)

O4 ^{iv} —Sr1—O5 ⁱⁱⁱ	76.1 (3)	Sr1 ^{xi} —O3—C12	157.0 (6)
O4 ^{iv} —Sr1—O6 ⁱⁱ	75.8 (3)	Sr1 ^{ix} —O4—C12	153.3 (6)
O4 ^{iv} —Sr1—O7 ⁱ	67.6 (3)	Sr1 ^{viii} —O5—C11	125.1 (4)
O4 ^{iv} —Sr1—O8	71.2 (4)	Sr1 ⁱⁱ —O6—C11	142.2 (5)
O5 ⁱⁱⁱ —Sr1—O6 ⁱⁱ	70.9 (4)	Sr1 ^{vii} —O7—C11	156.2 (7)
O5 ⁱⁱⁱ —Sr1—O7 ⁱ	114.04 (3)	Sr1—O8—C11	153.9 (7)

Symmetry codes: (i) $x, -y+1/2, z-1/2$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, y+1/2, -z+1/2$; (iv) $-x+1/2, -y+1, z-1/2$; (v) $x+1/2, -y+1/2, -z+1$; (vi) $x+1/2, y, -z+1/2$; (vii) $x, -y+1/2, z+1/2$; (viii) $-x+1, y-1/2, -z+1/2$; (ix) $-x+1/2, -y+1, z+1/2$; (x) $x-1/2, -y+1/2, -z+1$; (xi) $x-1/2, y, -z+1/2$.